

A Cartesian grid finite volume method for elliptic equations with variable coefficients and embedded interfaces

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Abstract

We present a finite volume method for the solution of the two-dimensional elliptic equation $\nabla \cdot (\beta(\mathbf{x})\nabla u(\mathbf{x})) = f(\mathbf{x})$ with variable, discontinuous coefficients and solution discontinuities on irregular domains. The method uses bilinear ansatz functions on Cartesian grids for the solution $u(\mathbf{x})$ resulting in a compact nine-point stencil. The resulting linear problem has been solved with a standard multigrid solver. Singularities associated with vanishing partial volumes of intersected grid cells or the dual bilinear ansatz itself are removed by a two-step asymptotic approach. The method achieves second order of accuracy in the L^∞ and L^2 norm.

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1. Introduction

We seek solutions of the two-dimensional variable coefficient elliptic equation

$$\nabla \cdot (\beta(\mathbf{x})\nabla u(\mathbf{x})) = f(\mathbf{x}), \quad \mathbf{x} \in \overline{\Omega} \setminus \Gamma \quad (1)$$

defined in a domain $\overline{\Omega} \setminus \Gamma$ with an embedded interface Γ . For simplicity we assume $\overline{\Omega}$ to be a simple rectangle. The embedded interface Γ separates two disjoint sub-domains $\overline{\Omega}^+$ and $\overline{\Omega}^-$ with $\overline{\Omega} = (\overline{\Omega}^+ \cup \overline{\Omega}^-) \setminus \Gamma$, see Fig. 1 for an illustration. Along the interface we prescribe jump conditions for the solution

$$[u]_\Gamma = u^+(\mathbf{x}) - u^-(\mathbf{x}) = g(\mathbf{x}_\Gamma) \quad (2)$$

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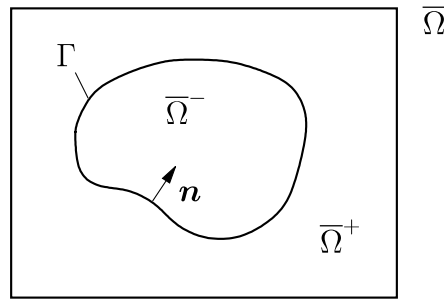


Fig. 1. Domain $\bar{\Omega}$ with sub-domains $\bar{\Omega}^+$, $\bar{\Omega}^-$, and embedded interface Γ .

and for its gradient in the normal direction

$$[\beta u_n]_\Gamma = \beta^+ u_n^+ - \beta^- u_n^- = h(\mathbf{x}_\Gamma), \quad (3)$$

with the notation $u_n = (\nabla u \cdot \mathbf{n})$. The unit normal vector \mathbf{n} on Γ is defined to point from $\bar{\Omega}^+$ to $\bar{\Omega}^-$.

Elliptic equations of type (1) with variable and discontinuous coefficients and solution discontinuities often arise as a component in modelling physical problems with embedded boundaries. Examples include incompressible two-phase flow with surface tension featuring jumps in pressure and pressure gradient across the interface, projection methods for zero Mach-number premixed combustion with jumps in the dynamic pressure and pressure gradient across the flame front, heat conduction between materials of different heat capacity and conductivity and interface diffusion processes. In the literature one can find a number of different approaches for the numerical solution of this type of problem. We limit our discussion here to methods on fixed Cartesian grids.

In Peskin's immersed boundary method [17], singular forces arising from discontinuous coefficients and jump conditions are treated as delta functions. Using discretised discrete delta functions, the discontinuity is spread over several grid cells making the method first-order accurate. The method has been used for many problems in mathematical biology and fluid mechanics. Recent work by Tornberg and Engquist [19,20,2] generalizes this approach and allows for high order approximations with minimal distribution of discontinuities or singular source terms over the computational grid.

Mayo [13,14] presented a second order accurate method for Poisson's equation and the biharmonic equation on irregular domains using an integral equation formulation. The resulting Fredholm integral equations of the second kind are solved with a fast Poisson solver on a rectangular region. Although the method captures solution discontinuities at the embedded interface, continuous derivatives have been assumed to evaluate the discrete Laplacian. The method can easily be extended to fourth order accuracy.

The immersed interface method [6–8] is a second order finite difference method on Cartesian grids for second order elliptic and parabolic equations with variable coefficients. Discontinuities in the solution and the normal gradient at the interface are explicitly incorporated into the finite difference stencil. Second order has been achieved by including additional points near the interface into the standard 5-point stencil leading to a non-standard six-point stencil in 2D. The resulting linear equation system is sparse but not symmetric or positive definite. Based on the immersed interface method Li and Ito [9] present a second order finite difference method which satisfies the sign property on the matrix coefficients which guarantees the discrete maximum principle. The resulting linear system of equations is non-symmetric but diagonally dominant and its symmetric part is negative definite.

A first order finite difference method on Cartesian grids was presented by Liu et al. [11]. Interface jump conditions are explicitly incorporated into the finite difference stencil as in the immersed interface method. Applying a one-dimensional approach in each spatial direction by implicitly smearing out the gradient jump condition, standard stencils (5-point in 2D, 9-point in 3D) for the discrete Laplacian are achieved leading to a symmetric positive definite matrix for the Poisson equation. The method shows first order accuracy for the solution u in the L^∞ -norm for constant coefficients β^\pm . A convergence proof of the method has been provided in [12] based on the weak formulation of the problem.

A finite element method on triangular meshes for solving second order elliptic and parabolic equations for interface problems with $[u] = 0$ and $[\beta u_n] \neq 0$ has been proposed by Chen and Zou [1]. In their method the triangles are aligned with the interface. In the L^2 -norm nearly second order accuracy ($h^2 |\log h|$) has been proved. The resulting linear system of equations is symmetric and positive definite. Another finite element method based on uniform triangulations of Cartesian grids was presented by Li et al. [10]. In contrast to [1], the triangles need not to be aligned with the interface. Numerical results with non-conforming finite elements demonstrate slightly less than second order of accuracy in L^∞ and second order of accuracy with conforming finite elements for a problem with homogeneous jump conditions $[u] = 0$, $[\beta u_n] = 0$. The general case with variable coefficients and non-homogeneous interface conditions $[u] \neq 0$, $[\beta u_n] \neq 0$ has been tackled recently by Hou and Liu [4] with a finite element method. Similar to [10] they use uniform triangulations of Cartesian grids. Their method is second order accurate in L^∞ if the solution u is C^2 and the interface is C^2 or C^1 .

Johansen and Colella [5] developed a second-order finite volume method on Cartesian grids for the variable coefficient Poisson equation on irregular domains with Dirichlet and Neumann boundary conditions and combined the method with an adaptive mesh refinement. Using central differencing for the gradients, their method reproduces the standard five-point stencil on regular cells. Using linear interpolation of gradients for internal edges and quadratic polynomials in normal direction to the boundary for irregular cells leads to a non-standard stencil. The final linear system is non-symmetric. Although remotely related to our work in the sense of using a finite volume method, the authors did not consider embedded boundaries with jump conditions of the solution and the normal derivative.

In this paper we present a second order finite volume method on Cartesian grids for solving the variable coefficient elliptic equation (1) with embedded interfaces and interface discontinuities. The motivation for a finite volume approach stems from our interest in conservative finite volume projection methods for Zero- and Low-Mach-number flow. The divergence constraint of the velocity field in a natural way leads to an elliptic equation for the pressure in a finite volume form. The use of piecewise bilinear ansatz function for the solution u makes our method quite similar to finite element methods and allows us to construct improved exact projection methods [21]. In two space dimensions the resulting system of linear equations is assembled from compact 9-point stencils. Compared to the cited literature our method differs in the following points: (i) we use a finite volume method instead of finite difference [6,11] or finite elements [4,10]; (ii) compared to the second order immersed interface method [6] we achieve always automatically a compact 9-point stencil without explicit incorporation of additional points near the interface or solution of an optimization problem as in [9]; (iii) instead of piecewise linear ansatz-functions on triangles as in the cited finite element methods we use piecewise bilinear ansatz-functions on the Cartesian grid. Compared to the finite element method presented in [4], we are able to construct a bilinear finite element which does not develop singularities when the element degenerates, e.g. for vanishing partial volumes of intersected cells. In contrast to the cited finite element methods our methods results in a non-symmetric matrix. In case of constant and equal coefficients we have a symmetric and positive definite matrix. In addition to representing a novel finite volume scheme for an important class of elliptic problems with embedded interfaces, our ideas and results may also be of value in the context of finite element methods on quadrilateral grids.

2. Finite volume formulation

Integrating Eq. (1) over an arbitrary control volume $\Omega \in \bar{\Omega}$ leads to

$$\int_{\Omega} \nabla \cdot (\beta \nabla u) dV = \int_{\Omega} f dV.$$

For a control volume $\Omega = \Omega^+ \cup \Omega^-$ intersected by the interface we obtain after applying the divergence theorem

$$\int_{\partial \Omega} \beta \nabla u \cdot \mathbf{n} dS = \int_{\Omega} f dV - \int_{\Gamma_{\Omega}} [\beta u_n] dS, \quad (4)$$

where Γ_Ω denotes the part of the embedded interface Γ lying inside Ω and $\partial\Omega = (\partial\Omega^+ \cup \partial\Omega^-) \setminus \Gamma_\Omega$. For $\Gamma_\Omega \neq \emptyset$ we have

$$\int_\Omega f \, dV = \int_{\Omega^+} f^+ \, dV + \int_{\Omega^-} f^- \, dV. \tag{5}$$

For a regular control volume without an embedded interface we have either $\Omega = \Omega^+ \in \overline{\Omega}^+ \wedge \Omega^- \equiv \emptyset$ or $\Omega = \Omega^- \in \overline{\Omega}^- \wedge \Omega^+ \equiv \emptyset$ and the last integral on the right side of (4) vanishes.

3. Numerical method

We discretise (4) on a uniform Cartesian grid in two-dimensional space. Let $\Delta x, \Delta y$ be the grid spacing in x and y -direction, see Fig. 2. The values $u_{i,j}$ of our discretised solution are located at the grid nodes with the coordinates $x_{i,j} = x_0 + i\Delta x, y_{i,j} = y_0 + j\Delta y$. The control volumes $\Omega_{i,j}$ are centered around the corresponding grid nodes i,j having edges of length Δx and Δy . Let $\mathfrak{N}_{i,j}$ be the set of rectangles – called cells in this work – adjacent to node i,j (I–IV in Fig. 2). The discrete form of (4) for the control volume $\Omega_{i,j}$ now reads as

$$\sum_{N \in \mathfrak{N}_{i,j}} \sum_{i=1}^2 \int_{l_i^N} \beta \nabla u \cdot \mathbf{n} \, dS = \int_{\Omega_{i,j}} f \, dV - \int_{\Gamma_{\Omega_{i,j}}} [\beta u_n] \, dS, \tag{6}$$

where $l_i^N, i = 1, 2$ are the two boundary edges with normals \mathbf{n}_1 and \mathbf{n}_2 of $\partial\Omega_{i,j}$ lying inside N .

To evaluate the left hand side of (6) we use a finite element approach with piecewise bilinear ansatz functions for u on each rectangular cell $N \in \mathfrak{N}_{i,j}$.

3.1. Bilinear finite elements for regular cells

For any regular cell $N \in \mathfrak{N}_{i,j}$ without embedded interface we apply a standard bilinear local ansatz

$$u(\xi, \eta) = c_0 + c_1\xi + c_2\eta + c_3\xi\eta, \quad \xi = \frac{x - x_0^N}{\Delta x}, \quad \eta = \frac{y - y_0^N}{\Delta y},$$

with $\xi, \eta \in [0, 1]$. Here, (x_0^N, y_0^N) denotes the origin of the local ξ, η -coordinate system in global (x, y) -space. The four unknown coefficients are uniquely determined by the four corner values of u . Given the piecewise bilinear distribution of $u(\xi, \eta)$ we evaluate the boundary integrals on the left side of (6) analytically. As an example, we have for upper integral of cell IV in Fig. 2

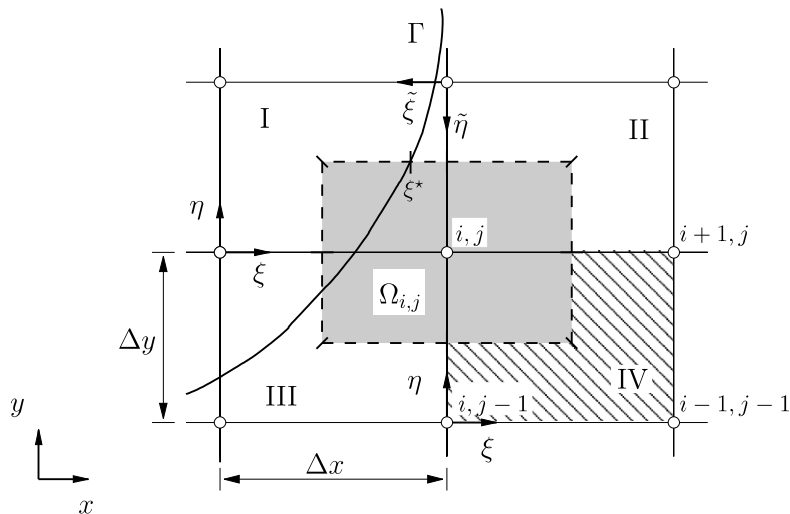


Fig. 2. Control volume $\Omega_{i,j}$. Discrete solution values are located at the grid nodes marked with circles. Regular cells II, IV, irregular cells I, III.

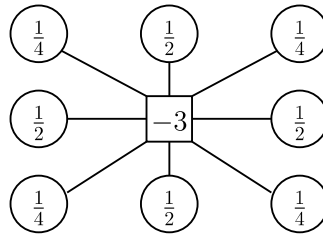


Fig. 3. Stencil weights of the discrete Laplacian for a regular cell with $\beta = 1$, $\Delta x = \Delta y$ using piecewise bilinear ansatz functions.

$$\int_{\Gamma_i^N} \beta \nabla u \cdot \mathbf{n} dS = \int_{0.5}^1 \beta \frac{\partial u}{\partial \xi} d\eta = \beta \frac{\Delta y}{\Delta x} \left(\frac{3}{8} (u_{i+1,j} - u_{i,j}) + \frac{1}{8} (u_{i+1,j-1} - u_{i,j-1}) \right). \tag{7}$$

Integrating over the whole boundary of $\Omega_{i,j}$ we find in the special case $\beta = 1$, $\Delta x = \Delta y$ the stencil elements for the discrete Laplacian of a regular control volume as displayed in Fig. 3. This discretization has been analyzed by Süli [18], who proved stability and second order convergence of the scheme on grids with arbitrary aspect ratio $\Delta x/\Delta y$.

3.2. Evaluation of source terms

For a second order approximation of (5) we use

$$\int_{\Omega} f dV = |\Omega^+| f^+(\mathbf{x}_s^+) + |\Omega^-| f^-(\mathbf{x}_s^-), \tag{8}$$

where \mathbf{x}_s^\pm denotes the barycenter of Ω^\pm .

To avoid additional computations of interface jump conditions, the boundary integral on the right hand side of (6) is evaluated assuming linear distributions of the interface jump conditions within cells. For a second order approximation we have

$$\int_{\Gamma_{\Omega_{i,j}}} [\beta u_n] dS = \sum_{N \in \mathfrak{N}_{i,j}} [\beta u_n] l_{\Gamma_{\Omega_{i,j}}^N}, \tag{9}$$

where $l_{\Gamma_{\Omega_{i,j}}^N}$ is the part of the interface $\Gamma_{\Omega_{i,j}}$ in cell N which belongs to the control volume $\Omega_{i,j}$.

3.3. Evaluation of the discrete Laplacian on irregular control volumes

In two spatial dimensions on a Cartesian grid, irregular cells can always be mapped onto one of the two unit-square cells shown in Figs. 4 and 6. We call a cell with an interface cutting the two adjacent edges of the upper right corner type I and type II otherwise. The position of the interface is assumed to be a piecewise straight line within the cell and is given by the zero level set of a signed normal distance function $\phi(\mathbf{x})$. On each side of the interface we make a bilinear ansatz:

$$\begin{aligned} u^{(\mathfrak{R})}(\xi, \eta) &= a_0 + a_1 \xi + a_2 \eta + a_3 \xi \eta, & \xi, \eta \in \Omega^{\mathfrak{R}}, \\ u^{(\mathfrak{S})}(\tilde{\xi}, \tilde{\eta}) &= b_0 + b_1 \tilde{\xi} + b_2 \tilde{\eta} + b_3 \tilde{\xi} \tilde{\eta}, & \tilde{\xi}, \tilde{\eta} \in \Omega^{\mathfrak{S}}. \end{aligned} \tag{10}$$

The gradients follow immediately

$$\begin{aligned} \frac{\partial u^{(\mathfrak{R})}}{\partial \xi} &= a_1 + a_3 \eta, & \frac{\partial u^{(\mathfrak{R})}}{\partial \eta} &= a_2 + a_3 \xi, \\ \frac{\partial u^{(\mathfrak{S})}}{\partial \tilde{\xi}} &= b_1 + b_3 \tilde{\eta}, & \frac{\partial u^{(\mathfrak{S})}}{\partial \tilde{\eta}} &= b_2 + b_3 \tilde{\xi}. \end{aligned} \tag{11}$$

The procedure of obtaining the eight unknown coefficients

$$\underline{x} = [a_0, a_1, a_2, a_3, b_0, b_1, b_2, b_3]^t \quad (12)$$

is given in detail below. However, we will always be able to write \underline{x} as a linear combination of the four unknown corner values u_i , $i = 1, \dots, 4$ and four known jump conditions $[u]_A$, $[u]_B$, $[\beta u_n]_A$, and $[\beta u_n]_B$:

$$\underline{x} = \underline{A} \underline{b}, \quad (13)$$

with $b = [u^t, [\cdot]^t]^t$, $\underline{u} = [u_1, u_2, u_3, u_4]^t$, and $[\cdot]^t = [[u]_A, [u]_B, [\beta u_n]_A, [\beta u_n]_B]^t$. Furthermore, using (11) we can evaluate any integral on the left hand side of (6) analytically on each irregular (and regular) cell. With (13) we can further express each of these integrals as a linear combination of the four unknown corner values and known jump conditions of the irregular cell. As an example, we consider cell I of the control volume $\Omega_{i,j}$ in Fig. 2, which is an irregular cell of type II, see Fig. 6. For boundary edge l_1^I with unit normal $\mathbf{n} = [n_x, n_y]^t = [0, 1]^t$ we can write

$$\begin{aligned} \int_{l_1^I} \beta \frac{\partial u}{\partial y} dx &= \frac{\Delta x}{\Delta y} \left(\int_{1/2}^{\xi^*} \beta^{21} \frac{\partial u^{21}}{\partial \eta} d\xi + \int_{\xi^*}^0 \beta^{23} \frac{\partial u^{23}}{\partial \tilde{\eta}} d\tilde{\xi} \right) \stackrel{(11)}{=} \frac{\beta^{21} \Delta x}{\Delta y} \left(a_2 \left(\xi^* - \frac{1}{2} \right) + a_3 \left(\frac{\xi^{*2}}{2} - \frac{1}{8} \right) \right) \\ &\quad - \frac{\beta^{23} \Delta x}{\Delta y} \left(b_2 \tilde{\xi}^* + b_3 \frac{\tilde{\xi}^{*2}}{2} \right) \\ &= \underline{D}_1 \underline{u} + \underline{D}_2 [\cdot], \end{aligned}$$

with $\underline{u} = [u_{i-1,j}, u_{i,j}, u_{i,j+1}, u_{i-1,j+1}]^t$. Going from the first to the second line we have introduced the gradients given in Eq. (11) and evaluated the integrals analytically. The matrices \underline{D}_1 and \underline{D}_2 are analytically deduced from \underline{A} and ξ^* and they contain only geometric information about the interface within the irregular cell I. Now, \underline{D}_1 determines the stencil coefficients for the discrete Laplacian, whereas $\underline{D}_2 [\cdot]$ will modify the right hand side of the discretised equation (6). Furthermore, as \underline{u} only contains the four unknown solution values, we will always obtain a compact nine-point stencil (except for corner or boundary points of $\bar{\Omega}$, where we have four or six-point stencils, respectively) during the calculation of the complete boundary integral on the left hand side of (6). We treat the coefficients β^{21} and β^{23} piecewise constant on each cell with values evaluated at the barycenters of the corresponding sub-areas. This procedure is in accordance with [4] and does not seem to effect the second order of the method. However, it is also possible to evaluate the coefficients either in the midpoint of each integral or to prescribe a distribution and doing the integration again analytically.

3.4. Piecewise bilinear finite elements for irregular cells

Using piecewise bilinear ansatz functions (10) on irregular cells, we remark two important properties to get the eight unknown coefficients in \underline{x} :

Remark 3.1. Along a line parallel to any of the two coordinate axis, i.e. $\xi = \text{const.}$ or $\eta = \text{const.}$, we have a linear distribution of u . This allows us to prescribe at most two independent jumps in the solution across the interface, e.g. $[u]_A, [u]_B$ in Figs. 4 and 6. If the interface is not parallel to a coordinate axis we can and do prescribe one additional jump $[u]_C$, whereas otherwise we can and do prescribe two of these jumps.

Remark 3.2. Along a line with $n_\xi = \pm n_\eta$ (i.e. the interface cuts the cell in a $\pm 45^\circ$ -angle), the gradient of u in normal direction $u_n = a_1 n_\xi + a_2 n_\eta + a_3 (\eta n_\xi + \xi n_\eta)$ is constant! In that case we can prescribe only one independent jump in the normal derivative, e.g. $[\beta u_n]_C$, Figs. 4 and 6.

A straightforward solution to determine the eight unknown coefficients would be to use the four corner values $\underline{u} = [u_1, u_2, u_3, u_4]^t$ complemented with jump conditions $[u]_A$, $[u]_B$, $[\beta u_n]_A$ and $[\beta u_n]_B$. However, it is obvious from Remark 3.2 that the resulting set of eight linear equations for \underline{x} has a singularity whenever $a = b$, $n_\xi = n_\eta = \frac{1}{\sqrt{2}}$ for cell type I as $[\beta u_n]_A$ and $[\beta u_n]_B$ are having the same set of coefficients in \underline{x} . The same singularity arises for cell type II if the interface crosses the cell diagonally.

Instead of using two jump conditions in $[\beta u_n]$, one could apply only one gradient jump condition with an additional jump in u , e.g. $[\beta u_n]_C$ and $[u]_C$, in the midpoint C of the interface, see Figs. 4 and 6. However, due to

Remark 3.1. $[u]_C$ becomes a linear combination of $[u]_A$ and $[u]_B$ whenever $a = b$ for type II and $b = 1, 0 \leq a < 1$ or $a = 1, 0 \leq b < 1$ for type I.

Another singularity arises for irregular cells of type I. For $a = b = 1$ the interface touches the cell through the upper right point of the cell. In that case the interface points A, B, C merge into one single point leading to identical equations in $[u]$ and $[\beta u_n]$.

The resulting set of linear equations for \underline{x} is not only unsolvable in any of the singular cases but the system becomes ill-conditioned in situations near the singularities. To remove all the discussed singularities, we propose a two-step asymptotic approach instead of trying to find the solution in a single step. Instead of (10) we set

$$\begin{aligned} u^{(\mathfrak{Q})}(\xi, \eta) &= u^{(\mathfrak{Q},0)}(\xi, \eta) + \varepsilon u^{(\mathfrak{Q},1)}(\xi, \eta), \\ u^{(\mathfrak{B})}(\tilde{\xi}, \tilde{\eta}) &= u^{(\mathfrak{B},0)}(\tilde{\xi}, \tilde{\eta}) + \varepsilon u^{(\mathfrak{B},1)}(\tilde{\xi}, \tilde{\eta}), \end{aligned} \tag{14}$$

with a properly defined small parameter ε . The functions $u^{(\mathfrak{Q},0)}, u^{(\mathfrak{Q},1)}, u^{(\mathfrak{B},0)}$, and $u^{(\mathfrak{B},1)}$ will be constructed in such a way that the resulting solution is identical to the single step solution (10) in all non-singular situations. Our base solution will be a solution satisfying the interface conditions $[u]_A, [u]_B, [u]_C$, and $[\beta u_n]_C$.

3.4.1. A bilinear finite element for irregular cell type I

In order to avoid the singularity discussed in Remark 3.2 we introduce an additional point C in the middle of the interface, see Fig. 4. We prescribe jump conditions $[u]_A, [u]_B, [u]_C = ([u]_A + [u]_B)/2$, and $[\beta u_n]_C = ([\beta u_n]_A + [\beta u_n]_B)/2$. The small parameter ε in (14) is defined as

$$\varepsilon = \min(\tilde{a}, \tilde{b}).$$

To capture all singular cases $\varepsilon = 0$ with the same leading order solution we need to define

$$\begin{aligned} [u]_A &= [u]_B, \quad \text{if } \varepsilon = 0 \quad \text{and } \tilde{b} = 0, \\ [u]_B &= [u]_A, \quad \text{if } \varepsilon = 0 \quad \text{and } \tilde{a} = 0. \end{aligned} \tag{15}$$

With this definition, we achieve that $u^{(\mathfrak{Q},0)}(1, 1) = u_3 - [u]_C$ for $\varepsilon = 0$. We define the leading order solution to be constant in region \mathfrak{B} and bilinear in \mathfrak{Q} :

$$\begin{aligned} u^{(\mathfrak{Q},0)}(\xi, \eta) &= a_0^{(0)} + a_1^{(0)}\xi + a_2^{(0)}\eta + a_3^{(0)}\xi\eta, \\ u^{(\mathfrak{B},0)}(\tilde{\xi}, \tilde{\eta}) &= b_0^{(0)}. \end{aligned} \tag{16}$$

For the coefficients we get $a_0^{(0)} = u_1, a_1^{(0)} = u_2 - u_1, a_2^{(0)} = u_4 - u_1, a_3^{(0)} = u_1 - u_2 + u_3 - u_4 + [u]_C$, and $b_0^{(0)} = u_3$. Including the zero valued coefficients on \mathfrak{B} we can write this as

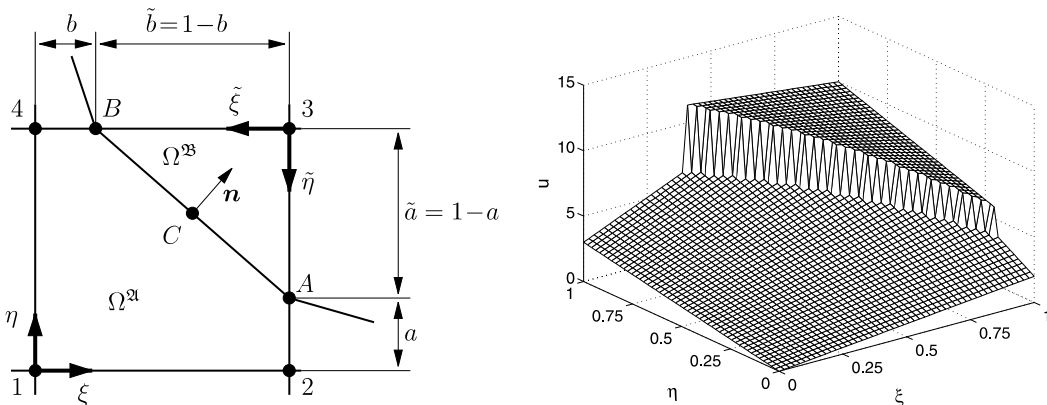


Fig. 4. Irregular cell type I in the local $\xi - \eta$ system with $\xi, \eta \in [0, 1]$ (left). Typical solution for $a = 0.2, b = 0.4, \beta^{\mathfrak{Q}} = 1, \beta^{\mathfrak{B}} = 1000, u_1 = 0, u_2 = 2, u_3 = 10, u_4 = 3, [u]_A = -2, [u]_B = -5, [\beta u_n]_A = 10, [\beta u_n]_B = 10$ (right).

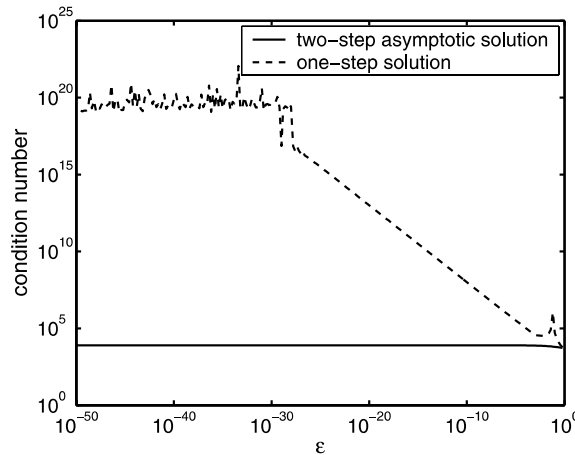


Fig. 5. Condition number of matrix $\underline{\underline{A}}^{(1)}$ in comparison with the resulting matrix from a one-step solution and a ratio $\beta^{2l}/\beta^{3l} = 1000$.

$$\underline{\underline{x}}^{(0)} = \left(\underline{\underline{A}}^{(0)}\right)^{-1} \underline{\underline{b}} \tag{17}$$

with

$$\underline{\underline{x}}^{(0)} = \begin{bmatrix} a_0^{(0)} \\ a_1^{(0)} \\ a_2^{(0)} \\ a_3^{(0)} \\ b_0^{(0)} \\ b_1^{(0)} \\ b_2^{(0)} \\ b_3^{(0)} \end{bmatrix}, \quad \left(\underline{\underline{A}}^{(0)}\right)^{-1} = \left[\begin{array}{cccc|cccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & -1 & 1 & -1 & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \dots & & & \dots & 0 & & \\ \vdots & & & & & & \vdots & \\ 0 & \dots & & & \dots & 0 & & \end{array} \right], \quad \underline{\underline{b}} = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ [u]_A \\ [u]_B \\ [\beta u_n]_A \\ [\beta u_n]_B \end{bmatrix} \tag{18}$$

Remark 3.3. Using (15), the leading order solution is the correct solution $u^{2l} = u^{(2l,0)}$ in the limit $\varepsilon = 0$. We note that the constant solution $u^{(3,0)}$ does not cover any gradient $u^{(3,0)}$ for $\varepsilon = 0$, $\tilde{a} \neq 0$ or $\varepsilon = 0$, $\tilde{b} \neq 0$. However, in those cases the interface is aligned with the boundary of the cell and the solution in region \mathfrak{B} does not have any influence on the evaluation of (6).

With the leading order solutions $u^{(2l,0)}$ and $u^{(3,0)}$ we proceed to the first correction which is in our linear problem already the exact final solution. We make a full bilinear ansatz on both sides of the interface:

$$\begin{aligned} u^{(2l,1)}(\xi, \eta) &= a_0^{(1)} + a_1^{(1)}\xi + a_2^{(1)}\eta + a_3^{(1)}\xi\eta, \\ u^{(3,1)}(\tilde{\xi}, \tilde{\eta}) &= b_0^{(1)} + b_1^{(1)}\tilde{\xi} + b_2^{(1)}\tilde{\eta} + b_3^{(1)}\tilde{\xi}\tilde{\eta}, \end{aligned} \tag{19}$$

where we have introduced a re-scaling

$$\hat{\xi} = \frac{\tilde{\xi}}{\tilde{b}}, \quad \hat{\eta} = \frac{\tilde{\eta}}{\tilde{b}}.$$

in region \mathfrak{B} . As the leading order solution covers already the four corner values of u , we get immediately $a_0^{(1)} = a_1^{(1)} = a_2^{(1)} = b_0^{(1)} = 0$. The missing four conditions for the remaining unknowns are the four jump conditions $[u]_A^{(1)}$, $[u]_B^{(1)}$, $[u]_C^{(1)}$, and $[\beta u_n]_C^{(1)}$ at the interface, leading to the following set of equations:

$$\underline{\underline{x}}^{(1)} = \left(\underline{\underline{A}}^{(1)}\right)^{-1} \underline{\underline{b}}^{(1)}, \tag{20}$$

with

$$\underline{x}^{(1)} = \left[a_0^{(1)}, a_1^{(1)}, a_2^{(1)}, a_3^{(1)}, b_0^{(1)}, b_1^{(1)}, b_2^{(1)}, b_3^{(1)} \right]^t,$$

$$\underline{b}^{(1)} = \left[0, 0, 0, 0, [u]_A^{(1)}, [u]_B^{(1)}, [u]_C^{(1)}, \varepsilon [\beta u_n]_C^{(1)} \right]^t,$$

and

$$\underline{A}^{(1)} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & a & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & b & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & \frac{(1+a)(1+b)}{4} & 0 & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{4} \\ 0 & 0 & 0 & \frac{\varepsilon \beta^{2\alpha} n_\xi (1+a)}{2\Delta x} + \frac{\varepsilon \beta^{2\alpha} n_\eta (1+b)}{2\Delta y} & 0 & \frac{\varepsilon \beta^{2\alpha} n_\xi}{b\Delta x} & \frac{\varepsilon \beta^{2\alpha} n_\eta}{a\Delta y} & \frac{\varepsilon \beta^{2\alpha} n_\xi}{b2\Delta x} + \frac{\varepsilon \beta^{2\alpha} n_\eta}{a2\Delta y} \end{bmatrix}$$

The last row of (20) – namely the jump condition $[\beta u_n]_C^{(1)}$ – has been multiplied by ε to keep $\underline{A}^{(1)}$ non-singular in the limit $\varepsilon \rightarrow 0$. The non-zero elements of $\underline{b}^{(1)}$ are given by

$$[u]_A^{(1)} = \frac{[u]_A - [u]_A^{(0)}}{\varepsilon} = \frac{1}{\varepsilon} \left([u]_A - \left(a_0^{(0)} + a_1^{(0)} + a_2^{(0)} a + a_3^{(0)} a - b_0^{(0)} \right) \right),$$

$$[u]_B^{(1)} = \frac{[u]_B - [u]_B^{(0)}}{\varepsilon} = \frac{1}{\varepsilon} \left([u]_B - \left(a_0^{(0)} + a_1^{(0)} b + a_2^{(0)} + a_3^{(0)} b - b_0^{(0)} \right) \right),$$

$$[u]_C^{(1)} = \frac{[u]_C - [u]_C^{(0)}}{\varepsilon} = \frac{1}{\varepsilon} \left([u]_C - \left(a_0^{(0)} + a_1^{(0)} \frac{1+b}{2} + a_2^{(0)} \frac{1+a}{2} + a_3^{(0)} \frac{(1+a)(1+b)}{4} - b_0^{(0)} \right) \right),$$

$$\varepsilon [\beta u_n]_C^{(1)} = [\beta u_n]_C - [\beta u_n]_C^{(0)} = [\beta u_n]_C - \beta^{2\alpha} \left(a_1^{(0)} \frac{n_\xi}{\Delta x} + a_2^{(0)} \frac{n_\eta}{\Delta y} + a_3^{(0)} \left(\frac{n_\xi(1+a)}{2\Delta x} + \frac{n_\eta(1+b)}{2\Delta y} \right) \right).$$

Using the leading order solution (17) we can write $\underline{b}^{(1)}$ with (21) as

$$\underline{b}^{(1)} = \underline{B}_1 \underline{x}^{(0)} + \underline{B}_2 \underline{b} = \left(\underline{B}_1 \left(\underline{A}^{(0)} \right)^{-1} + \underline{B}_2 \right) \underline{b},$$

and further

$$\underline{x}^{(1)} = \left(\underline{A}^{(1)} \right)^{-1} \underline{b}^{(1)} = \left(\underline{A}^{(1)} \right)^{-1} \left(\underline{B}_1 \left(\underline{A}^{(0)} \right)^{-1} + \underline{B}_2 \right) \underline{b}. \tag{22}$$

The matrices \underline{B}_1 and \underline{B}_2 are introduced to write $\underline{b}^{(1)}$ in terms of $\underline{x}^{(0)}$ and \underline{b} . They follow directly from (21) and are listed in Appendix A.

The complete solution for an irregular cell type I can now be assembled using (14), (16), (17), (19) and (22):

$$\underline{x} = \underline{A} \underline{b} = \left(\left(\underline{A}^{(0)} \right)^{-1} + \varepsilon \left(\underline{A}^{(1)} \right)^{-1} \left(\underline{B}_1 \left(\underline{A}^{(0)} \right)^{-1} + \underline{B}_2 \right) \right) \underline{b}, \tag{23}$$

Eq. (23) requires to invert $\underline{A}^{(1)}$. Instead of using a two-step asymptotic approach one could calculate \underline{x} in a single step. However, the system becomes singular as $\varepsilon \rightarrow 0$ due to the exposed reasons. Fig. 5 compares the condition number of matrix $\underline{A}^{(1)}$ from the asymptotic two-step scheme with the resulting matrix of a single step as a function of the small parameter ε and a ratio $\beta^{2\alpha} / \beta^{2\beta} = 1000$. The condition number of the single-step solution quickly becomes extremely large. Our two-step asymptotic approach has an almost constant condition number for $\varepsilon \rightarrow 0$ and has a well defined solution for $\varepsilon = 0$. The singularity is shifted from the set of linear equations to the small parameter ε . In the numerical implementation we need to evaluate the term $1/\varepsilon$, see (21). We get clean solutions for ε as small as r_{\min} , where r_{\min} is the smallest positive floating point number ($r_{\min} = 2.2251 \times 10^{-308}$ for double precision floating point arithmetic on our machine). However, if $\varepsilon < \text{eps}^2$, where eps is the relative floating point accuracy, we set $\underline{x} = \underline{x}^{(0)}$ and $\underline{b} = \underline{b}^{(0)}$ and do not compute the next order solution. The asymptotic two-step solution is identical to the single-step solution with the exception that the asymptotic solution stays well behaved in the limit $\varepsilon \rightarrow 0$.

3.4.2. A bilinear finite element for irregular cell type II

The construction of a non-singular bilinear finite element for an irregular cell of type II, Fig. 6, follows the lines presented in the preceding section for type I. Again, our base solution will be constructed with three prescribed solution jumps $[u]$ and one gradient jump $[\beta u_n]$ across the interface. This ensures identical solutions for type I and type II cells under conditions $a = 0, b \in [0, 1]$ for type I and $a = 1, b \in [0, 1]$ for type II, respectively. However, as pointed out in Remark 3.1, we cannot prescribe three independent jump conditions $[u]$ if $a = b$, i.e., the interface cuts the cell perpendicular to the ξ -axis. To resolve this singularity we apply the two-step asymptotic approach (14) with the small parameter now defined as

$$\varepsilon = (a - b).$$

We use a bilinear ansatz function for the leading order solution on both sides of the interface

$$\begin{aligned} u^{(2l,0)}(\xi, \eta) &= a_0^{(0)} + a_1^{(0)}\xi + a_2^{(0)}\eta + a_3^{(0)}\xi\eta, \\ u^{(2s,0)}(\tilde{\xi}, \tilde{\eta}) &= b_0^{(0)} + b_1^{(0)}\tilde{\xi} + b_2^{(0)}\tilde{\eta} + b_3^{(0)}\tilde{\xi}\tilde{\eta}. \end{aligned} \tag{24}$$

The leading order solution is determined by the four corner values of u and the jump conditions $[u]_{\bar{A}}$, $[u]_{\bar{B}}$, $[\beta u_n]_{\bar{A}}$, and $[\beta u_n]_{\bar{B}}$. Points \bar{A} and \bar{B} are defined to have the same ξ -coordinate as point C , i.e. $\xi_{\bar{A}} = \xi_{\bar{B}} = \xi_C = (a + b)/2$, so that $\bar{A} = A$ and $\bar{B} = B$ in the limit $\varepsilon = 0$, see Fig. 6. Therefore, the imaginary leading order interface has a unit normal vector $\mathbf{n}^{(0)} = [1, 0]^t$. The coefficients $a_0^{(0)} = u_1, a_2^{(0)} = u_4 - u_1, b_0^{(0)} = u_3,$ and $b_2^{(0)} = u_2 - u_3$ are defined by the corner values. With a unit normal vector $\mathbf{n}^{(0)} = [1, 0]^t$ for the leading order solution we have quasi one-dimensional distributions of u along $\eta = \text{const.}$ lines. The solution for the remaining coefficients is (see also [11,16])

$$\begin{aligned} a_1^{(0)} &= \frac{\beta^{2s}}{\delta} \left(-u_1 + u_2 + [u]_A - \frac{(1-c)\Delta x}{\beta^{2s}} [\beta u_n]_A \right), \\ b_1^{(0)} &= \frac{-\beta^{2l}}{\delta} \left(-u_1 + u_2 + [u]_A + \frac{c\Delta x}{\beta^{2l}} [\beta u_n]_B \right), \\ a_3^{(0)} &= \frac{\beta^{2s}}{\delta} \left(u_1 - u_2 + u_3 - u_4 - [u]_A + [u]_B - \frac{(1-c)\Delta x}{\beta^{2s}} ([\beta u_n]_A - [\beta u_n]_B) \right), \\ b_3^{(0)} &= \frac{-\beta^{2l}}{\delta} \left(-u_1 + u_2 - u_3 + u_4 + [u]_A - [u]_B + \frac{(1-c)\Delta x}{\beta^{2l}} ([\beta u_n]_A - [\beta u_n]_B) \right), \end{aligned}$$

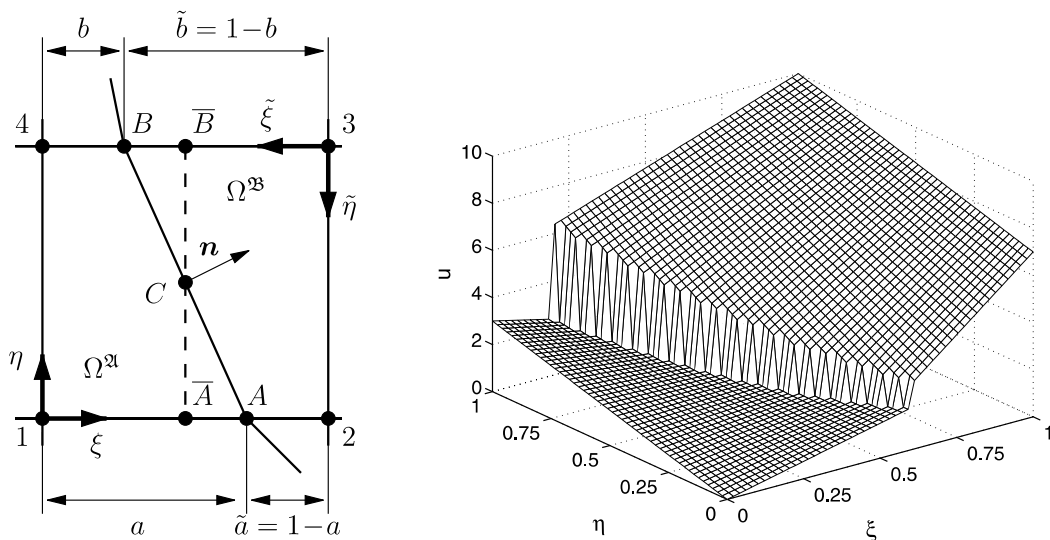


Fig. 6. Irregular cell type II in the local $\xi - \eta$ system with $\xi, \eta \in [0, 1]$ (left). Solution for $a = 0.6, b = 0.2, \beta^{2l} = 100, \beta^{2s} = 1, u_1 = 0, u_2 = 7, u_3 = 10, u_4 = 3, [u]_A = -1, [u]_B = -4, [\beta u_n]_A = 1, [\beta u_n]_B = 10$ (right).

with $\delta = \beta^{\mathfrak{B}}(a + b)/2 + \beta^{\mathfrak{A}}((1 - a) + (1 - b))/2$. For later purposes, we write the leading order solution in matrix form

$$\underline{x}^{(0)} = \left(\underline{A}^{(0)}\right)^{-1} \underline{b} \tag{25}$$

with

$$\underline{x}^{(0)} = \begin{bmatrix} a_0^{(0)} \\ a_1^{(0)} \\ a_2^{(0)} \\ a_3^{(0)} \\ b_0^{(0)} \\ b_1^{(0)} \\ b_2^{(0)} \\ b_3^{(0)} \end{bmatrix}, \quad \left(\underline{A}^{(0)}\right)^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\delta^{\mathfrak{A}} & \delta^{\mathfrak{A}} & 0 & 0 & \delta^{\mathfrak{A}} & 0 & \delta^{\mathfrak{A}}\gamma^{\mathfrak{A}} & 0 \\ -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ \delta^{\mathfrak{A}} & -\delta^{\mathfrak{A}} & \delta^{\mathfrak{A}} & -\delta^{\mathfrak{A}} & -\delta^{\mathfrak{A}} & \delta^{\mathfrak{A}} & -\delta^{\mathfrak{A}}\gamma^{\mathfrak{A}} & \delta^{\mathfrak{A}}\gamma^{\mathfrak{A}} \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \delta^{\mathfrak{B}} & -\delta^{\mathfrak{B}} & 0 & \delta^{\mathfrak{B}} & 0 & -\delta^{\mathfrak{B}}\gamma^{\mathfrak{B}} \\ 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 \\ -\delta^{\mathfrak{B}} & \delta^{\mathfrak{B}} & -\delta^{\mathfrak{B}} & \delta^{\mathfrak{B}} & \delta^{\mathfrak{B}} & -\delta^{\mathfrak{B}} & -\delta^{\mathfrak{B}}\gamma^{\mathfrak{B}} & \delta^{\mathfrak{B}}\gamma^{\mathfrak{B}} \end{bmatrix}, \tag{26}$$

$$\underline{b} = [u_1, u_2, u_3, u_4, [u]_A, [u]_B, [\beta u_n]_A, [\beta u_n]_B]^t,$$

and $\delta^{\mathfrak{A}} = \beta^{\mathfrak{B}}/\delta$, $\delta^{\mathfrak{B}} = -\beta^{\mathfrak{A}}/\delta$, $\delta = (\xi_C \beta^{\mathfrak{B}} + \tilde{\xi}_C \beta^{\mathfrak{A}})$, $\gamma^{\mathfrak{A}} = \frac{\tilde{\xi}_C \Delta x}{\beta^{\mathfrak{B}}}$, $\gamma^{\mathfrak{B}} = \frac{\xi_C \Delta x}{\beta^{\mathfrak{A}}}$. Furthermore, we define $[u]_C = ([u]_A + [u]_B)/2$.

We use a similar bilinear ansatz for the correction as in (19):

$$\begin{aligned} u^{\mathfrak{A},(1)}(\xi, \eta) &= a_0^{(1)} + a_1^{(1)}\xi + a_2^{(1)}\eta + a_3^{(1)}\xi\eta, \\ u^{\mathfrak{B},(1)}(\tilde{\xi}, \tilde{\eta}) &= b_0^{(1)} + b_1^{(1)}\tilde{\xi} + b_2^{(1)}\tilde{\eta} + b_3^{(1)}\tilde{\xi}\tilde{\eta}, \end{aligned} \tag{27}$$

where the leading order solution with (14) immediately yields $a_0^{(1)} = a_2^{(1)} = b_0^{(1)} = b_2^{(1)} = 0$. The remaining coefficients are calculated using the four jump conditions at the interface, with the first three of them

$$\begin{aligned} [u]_A^{(1)} &= \frac{[u]_A - [u]_A^{(0)}}{\varepsilon} = \frac{1}{\varepsilon} \left([u]_A - \left(a_0^{(0)} + a_1^{(0)}a - b_0^{(0)} - b_1^{(0)}\tilde{a} - b_2^{(0)} - b_3^{(0)}\tilde{a} \right) \right), \\ [u]_B^{(1)} &= \frac{[u]_B - [u]_B^{(0)}}{\varepsilon} = \frac{1}{\varepsilon} \left([u]_B - \left(a_0^{(0)} + a_1^{(0)}b + a_2^{(0)} + a_3^{(0)}b - b_0^{(0)} - b_1^{(0)}\tilde{b} \right) \right), \\ [\beta u_n]_C^{(1)} &= \frac{[\beta u_n]_C - [\beta u_n]_C^{(0)}}{\varepsilon} = \frac{1}{\varepsilon} \left([\beta u_n]_C - \beta^{\mathfrak{A}} \left(a_1^{(0)} \frac{n_\xi}{\Delta x} + a_2^{(0)} \frac{n_\eta}{\Delta y} + a_3^{(0)} \left(\frac{n_\xi}{2\Delta x} + \frac{n_\eta(a+b)}{2\Delta y} \right) \right) \right. \\ &\quad \left. - \beta^{\mathfrak{B}} \left(b_1^{(0)} \frac{n_\xi}{\Delta x} + b_2^{(0)} \frac{n_\eta}{\Delta y} + b_3^{(0)} \left(\frac{n_\xi}{2\Delta x} + \frac{n_\eta(\tilde{a} + \tilde{b})}{2\Delta y} \right) \right) \right). \end{aligned} \tag{28}$$

We do not want to use jump condition $[u]_C$ directly as we have $[u]_C^{(1)} \rightarrow ([u]_A^{(1)} + [u]_B^{(1)})/2$ in the limit $\varepsilon \rightarrow 0$ making the resulting equation a linear combination of the two other jump conditions. Instead, we use $[u]_C$ in the following form

$$\Delta[u] = [u]_C - \frac{1}{2}([u]_A + [u]_B) = -\varepsilon \left(\frac{a_3 - b_3}{4} \right).$$

This leads us to the fourth condition for the unknown coefficients:

$$\Delta[u]^{(1)} = [u]_C^{(1)} - \frac{1}{2}([u]_A^{(1)} + [u]_B^{(1)}) = \frac{\Delta[u] - \Delta[u]^{(0)}}{\varepsilon} = -\frac{a_3^{(0)} - b_3^{(0)}}{\varepsilon}. \tag{29}$$

Taking into account the known zero values of some of the coefficients, the complete set of linear equations can now be written as

$$\underline{x}^{(1)} = \left(\underline{A}^{(1)}\right)^{-1} \underline{b}^{(1)}$$

with

$$\underline{\underline{A}}^{(1)} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & a & 0 & 0 & 0 & -\tilde{a} & 0 & -\tilde{a} \\ 0 & b & 0 & b & 0 & -\tilde{b} & 0 & 0 \\ 0 & 0 & 0 & 1/4 & 0 & 0 & 0 & -1/4 \\ 0 & \frac{\beta^{2\alpha} n_\xi}{\Delta x} & 0 & \frac{\beta^{2\alpha} n_\xi}{2\Delta x} + \frac{\beta^{2\alpha} n_\eta (a+b)}{2\Delta y} & 0 & \frac{\beta^{2\alpha} n_\xi}{\Delta x} & \frac{\beta^{2\alpha} n_\xi}{2\Delta x} + \frac{\beta^{2\alpha} n_\eta (\tilde{a}+\tilde{b})}{2\Delta y} & 0 \end{bmatrix},$$

$$\underline{x}^{(1)} = [a_0^{(1)}, a_1^{(1)}, a_2^{(1)}, b_3^{(1)}, b_0^{(1)}, b_1^{(1)}, b_2^{(1)}, b_3^{(1)}]^t,$$

and

$$\underline{b}^{(1)} = [0, 0, 0, 0, [u]_A^{(1)}, [u]_B^{(1)}, \Delta[u]^{(1)}, [\beta u_n]_C^{(1)}]^t.$$

The non-zero elements of $\underline{b}^{(1)}$ are given by the right hand sides of (28) and (29). Instead of solving for $\underline{x}^{(1)}$ we solve directly for $\varepsilon \underline{x}^{(1)}$. Doing so, factors of $1/\varepsilon$ in (28) and (29) cancel and we do not need to divide by ε at any point for this type of element. With the leading order solution $\underline{x}^{(1)}$ and the correction $\varepsilon \underline{x}^{(1)}$ we assemble the complete solution following the lines presented in Section 3.4.1 and end with

$$\underline{x} = \underline{\underline{A}} \underline{b} = \left((\underline{\underline{A}}^{(0)})^{-1} + (\underline{\underline{A}}^{(1)})^{-1} (\underline{\underline{B}}_1 (\underline{\underline{A}}^{(0)})^{-1} + \underline{\underline{B}}_2) \right) \underline{b}. \tag{30}$$

The matrices $\underline{\underline{B}}_1$ and $\underline{\underline{B}}_2$ are again introduced to write the correction solution $\underline{b}^{(1)}$ in terms of $\underline{x}^{(0)}$ and \underline{b} and are provided in Appendix B.

Fig. 7 shows the condition number for matrix $\underline{\underline{A}}^{(1)}$ as a function of the parameter ε and compares it with the condition number of the matrix resulting from a one-step solution. The condition number in the two-step asymptotic scheme is almost independent of ε , whereas the condition number for the one-step solution scales inverse proportional to ε . We note that with increasing condition number the difference between the two-step asymptotic solution and the single-step increases making the one-step solution useless in the limit $\varepsilon \rightarrow 0$.

3.5. Numerical stability investigation

The matrix resulting from our discretisation scheme is non-symmetric in general and not diagonally dominant. This is true as well for the original immersed interface method [6]. The development of a formal stability

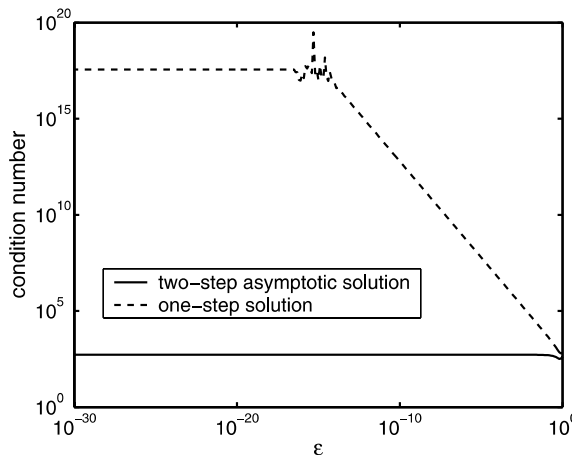


Fig. 7. Condition number of matrix $\underline{\underline{A}}^{(1)}$ in comparison with the resulting matrix from a one-step solution and a ratio $\beta^{2\alpha}/\beta^{2\beta} = 1000$.

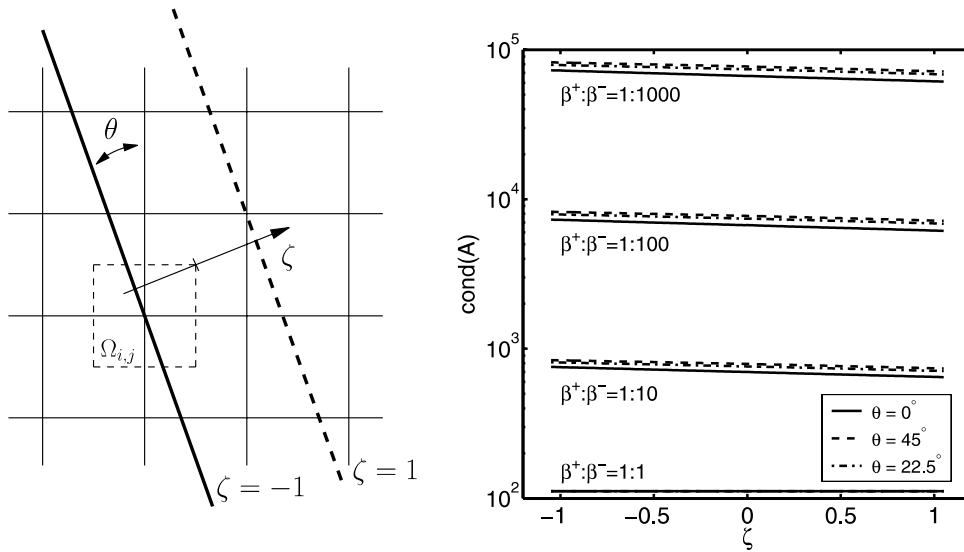


Fig. 8. Condition-number of the resulting matrix for different values of the coefficients β^+ and β^- as the interface moves over the grid with 16×16 nodes.

proof is a formidable task that is beyond the scope of this paper. Instead, we provide some representative numerical stability tests which indicate robustness of our discretisation.

A first stability test addresses the question of how the condition number of the resulting matrix is affected by the position of the interface relative to the underlying grid. Fig. 8 shows values of the condition number for different ratios of the coefficients β^+/β^- as we move a straight interface at different angles over one cell of the grid (here: 16×16 grid points on a computational domain $-1 \leq x, y \leq 1$). The condition number has been defined as the ratio of the largest to the smallest non-zero eigenvalue of the matrix and computed with the Matlab. Since we do not include any boundary conditions for this test, the resulting matrix is singular. Note, however, that the resulting matrix has always only a single zero eigenvalue associated with the undetermined absolute mean value of the solution. A value of $\zeta = -1$ corresponds to the first hit of the interface with the cell whereas at $\zeta = 1$ the interface hits the upper right corner, cf. Fig. 8. The interval $-1 \leq \zeta \leq 1$ has been resolved by 200 steps, i.e. 200 different positions of the interface.

The tests have been set up to cover all possible singularities associated with our dual bilinear ansatz. An angle $\theta = 0^\circ$ covers singularities pointed out in Remark 3.1, while $\theta = 45^\circ$ leads to the singularities of Remark 3.2. In the case of constant and equal coefficients $\beta^+:\beta^- = 1$ we see a constant condition number independent of the position of the interface. For this special – although non-trivial – case the stencil elements are identical to those in the case without interface (see Fig. 3), and the resulting matrix is symmetric and diagonally dominant.

Increasing the ratio of the coefficients increases the condition number linearly with the the ratio $\beta^+:\beta^-$. However, as seen in Fig. 8, the condition number changes very smoothly and weakly with the position of the interface relative to the underlying grid, and it exhibits no deviation in any of the singular cases.

A distinct feature in the theory of second order elliptic equations is their maximum principle. For any numerical method solving elliptic problems a discrete maximum principle is therefore a desirable feature beyond a reasonable order of convergence. Furthermore, if a numerical discretisation preserves a discrete maximum principle, it is relatively straightforward to rigorously prove stability and convergence [15].

For each discrete control volume $\Omega_{i,j}$, our finite volume method (6) leads to a 9-points stencil for the approximation of the discrete Laplacian:

$$\sum_{N \in \mathfrak{N}_{i,j}} \sum_{i=1}^2 \int_{I_i^N} \beta \nabla u \cdot \mathbf{n} dS \approx \mathfrak{L}_h u_{i,j} = \sum_{k=1}^8 \gamma_k u_k + \gamma_C u_C,$$

where C denotes the central stencil element and the sum over k is taken over all mesh points which are neighbors of C . A sufficient condition for a numerical discretisation to satisfy a discrete maximum principle is that

all stencil weights $\gamma_k > 0$, $\gamma_C < 0$, and $\sum_{k=1}^8 \gamma_k \leq |\gamma_C|$ (for details and additional assumptions see e.g. [15]). The stencil weights of our method in the case of a regular cell for constant coefficient β are given in Fig. 3. The related scheme satisfies a discrete maximum principle and has been proven by Süli [18] to be stable and second order accurate. In the case of constant and equal coefficients $\beta^+:\beta^- = 1$ our discretisation leads to the same stencil even for irregular cells. However, in the general case with $\beta^+:\beta^- \neq 1$ this is not the case and one cannot use standard arguments based on the stencil weights of single rows within the resulting matrix to argue for a discrete maximum principle. Fig. 9 shows maximum and minimum values for the off-diagonal stencil weights γ_k and the diagonal stencil weight γ_C for control volume $\Omega_{i,j}$ (Fig. 8) as we move the interface over a cell at two different angles and a ratio $\beta^+:\beta^- = 1:100$. It is apparent that the condition $\gamma_k > 0$ is not satisfied in general which is a potential sign of instability. There are at least the following two options to address this issue: (i) At those grid points, we can change to a lower order scheme locally, such as harmonic averaging, without affecting the global second order accuracy of the scheme. (ii) We are currently working on an extended scheme that addresses the limit of large or vanishing β through an asymptotic decomposition of the problem.

Here we provide a numerical test indicating that our method likely satisfies a discrete maximum principle. We consider a case with constant solution $u^+(\mathbf{x}) = 0$, $\mathbf{x} \in \Omega^+$ and $u^-(\mathbf{x}) = \zeta - \zeta_0 = x \cos(\theta) + y \sin(\theta) - \zeta_0$, $x, y \in \Omega^-$. We use the exact solution to compute values for Dirichlet boundary conditions, the jump condition $[\beta u_n]$ and the right hand side (5). The solution satisfies the condition $[u] \equiv 0$. Fig. 10 shows on the left side the numerical solution on a computational domain $-1 \leq x, y \leq 1$ with 16×16 grid points and a straight interface at an angle of 10° and a ratio $\beta^+:\beta^- = 1:1000$. If our stencil were to violate the maximum principle for this case we should observe values $u^+ > 0$. On the right side of Fig. 8 we display the maximum values of u on the computational domain as we move the front at different angles over one cell. The maximum value is always comparable the machine accuracy (more precisely, to the order of the convergence criteria of the linear equation solver). We have repeated this test with different ratios $\beta^+:\beta^-$ and in no case did we observe a violation of the discrete maximum principle.

We remark that it is very difficult to investigate the discrete maximum principle numerically with non-linear solutions u^- . The linear solution $u^-(\mathbf{x}) = \zeta - \zeta_0$ allows us to compute the interface source term (9) – and therefore the entire right hand side of the linear system of equations – exactly! If we cannot provide an exact right hand side, a violation of the maximum principle could be induced by the discretisation error of the right hand side terms. Additional numerical tests with more or less arbitrarily complex geometries and constant solutions in Ω^+ and Ω^- satisfied in all cases the discrete maximum principle.

We conclude from these tests that our method is a promising candidate for rigorous stability analysis. We defer such analysis, as well as a systematic asymptotic study for $\beta^+/\beta^- \rightarrow \infty$, to subsequent publications.

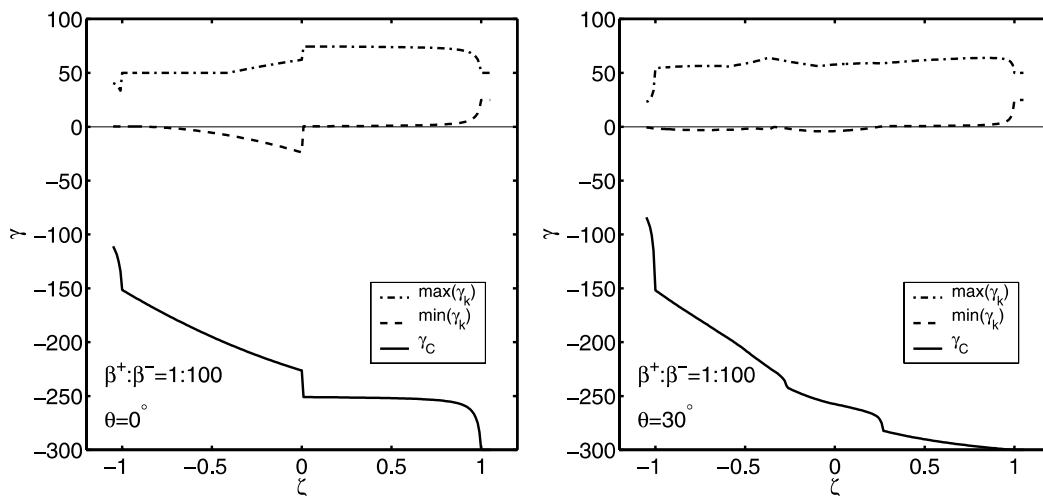


Fig. 9. Stencil weights γ of the discrete Laplacian for an irregular cell $\beta^+:\beta^- = 1:100$ as the interface moves over the cell (for definition of ζ and θ see Fig. 8).

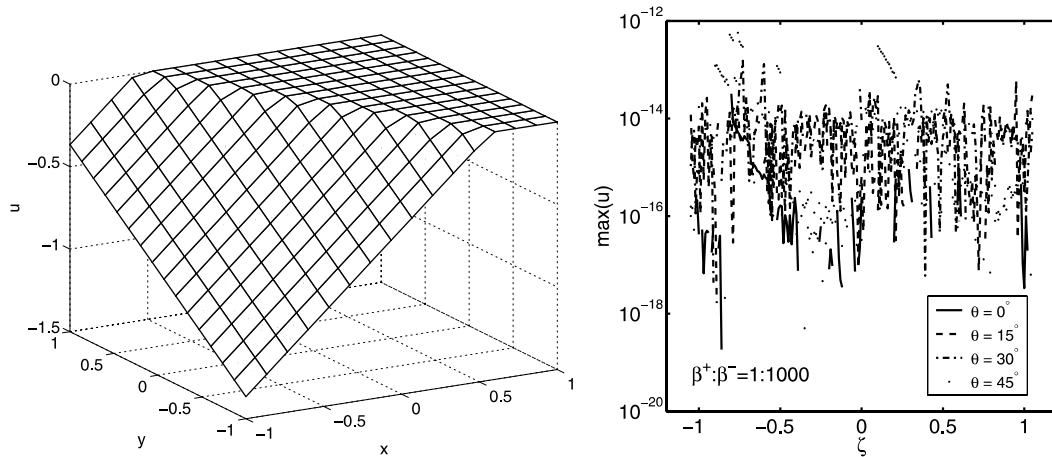


Fig. 10. Solution for the discrete maximum principle investigation on a 16×16 grid and a ratio $\beta^+:\beta^- = 1:1000$ (left). Maximum values of the solution u with variation of the position of the interface (right, for definition of ζ and θ see Fig. 8).

4. Numerical results

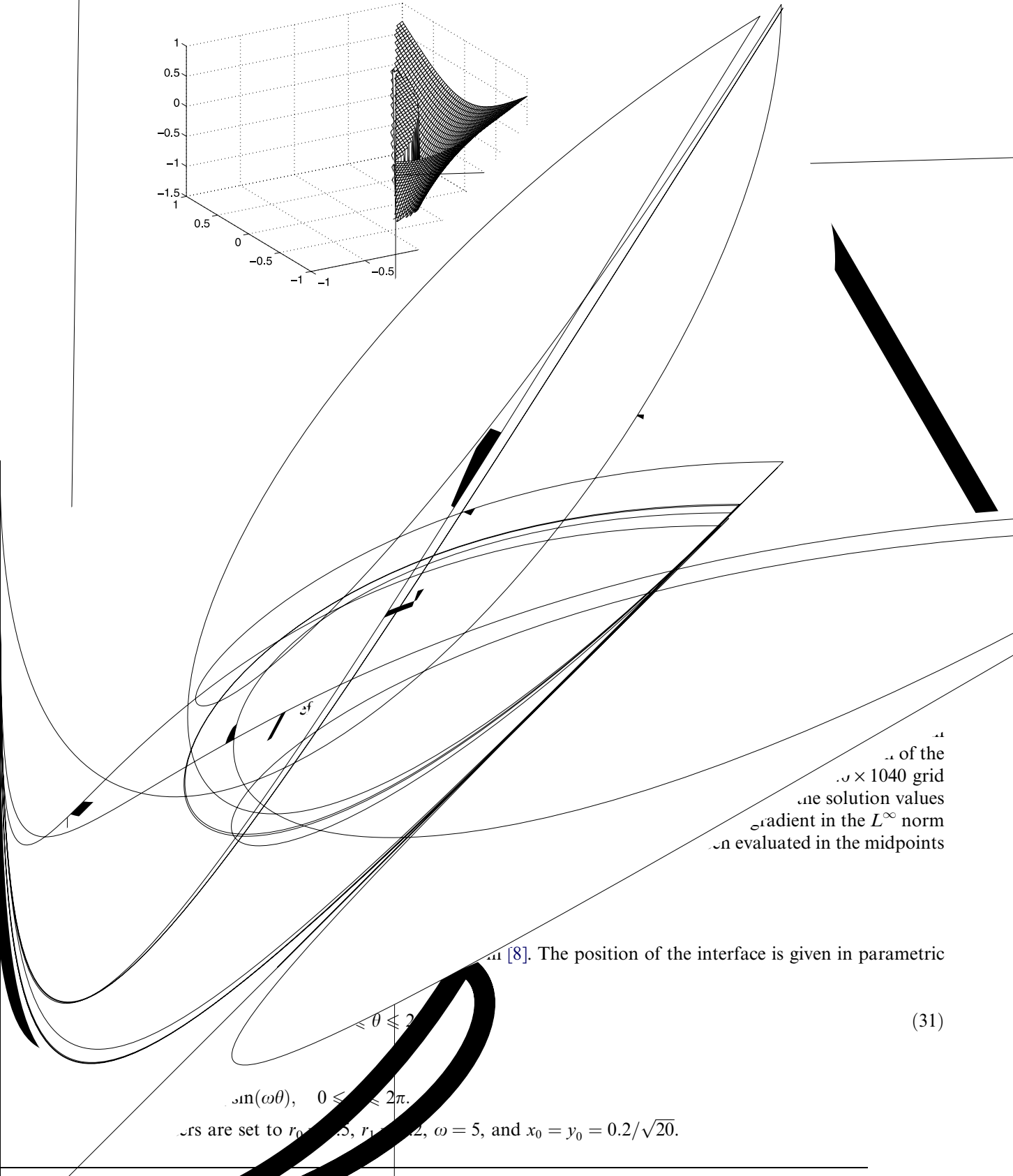
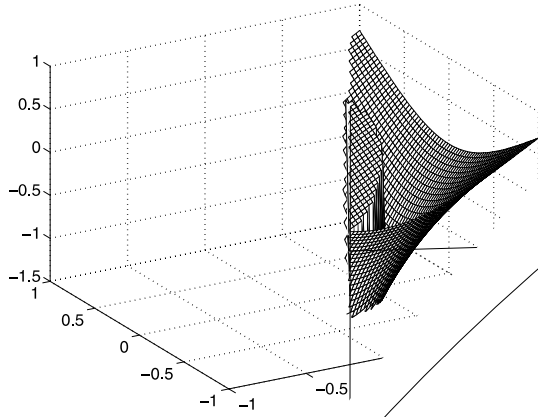
In following examples we compare numerical results with given analytic solutions $u^+(\mathbf{x})$ and $u^-(\mathbf{x})$ and corresponding coefficients $\beta^+(\mathbf{x})$ and $\beta^-(\mathbf{x})$. We use the analytic solution to provide the right hand side $f(\mathbf{x})$ in (1) and to prescribe jump conditions $[u]$ and $[\beta u_n]$ at positions where the interface Γ crosses grid lines. Furthermore, the analytic solution provides us with the proper Dirichlet boundary conditions. The interface is defined by the zero level of the signed normal distance function $\phi(\mathbf{x})$. We set Ω^+ and Ω^- to be the region with $\phi(\mathbf{x}) > 0$ and $\phi(\mathbf{x}) < 0$, respectively. The position of the interface has been evaluated assuming linear distributions of ϕ between grid points. The unit normal vector pointing from Ω^+ to Ω^- is given by $\mathbf{n} = -\frac{\nabla\phi}{|\nabla\phi|}$. The arising linear systems of equations have been solved with the hypre library [3] using an algebraic multigrid solver (AMG) or an AMG preconditioned BICGSTAB solver. In our examples we made the experience that the AMG solver works very reliable and fast up to a ratio of the coefficients β^+ and β^- of 1/100 and 100/1. For ratios of the coefficients of 1000 and above we were not able to get solutions with the AMG alone and used the AMG preconditioned BICGSTAB algorithm (see also our remarks on large coefficient ratios in the conclusions, Section 5).

4.1. Example 1

This example is taken from [4]. We solve (1) in the domain $-1 \leq x, y \leq 1$. The interface is a simple circle with radius 0.5 and midpoint at (0,0). The analytic solutions u^\pm , the coefficients β^\pm , and the level set function are given as follows:

$$\begin{aligned}
 u^+ &= \ln(x^2 + y^2), & u^- &= \sin(x + y), \\
 \beta^+ &= \sin(x + y) + 2, & \beta^- &= \cos(x + y) + 2, \\
 \phi &= \sqrt{(x^2 + y^2)} - 0.5.
 \end{aligned}$$

The solution as well as the the normal derivative are discontinuous across the interface. This example is characterized by a simple geometry of the interface and a small difference between the coefficients β^+ and β^- . Fig. 11 shows the numerical solution of the method using 80×80 grid-points. A convergence study with two different sets of grids – one with $\Delta x/\Delta y = 1$ and the other with $\Delta x/\Delta y = 3$ – is summarized in Table 1. The method achieves second order of accuracy in the L^2 , and L^∞ norm on both sets of grids. Our results are comparable to the ones presented in [4] with a smaller error constant reported in [4]. However, using triangulated Cartesian grids in [4], the interface is resolved with almost twice as many points as in our method on an identical underlying Cartesian grid. This example shows a smooth second order behavior for the error with



of the
 1024×1024 grid
 the solution values
 gradient in the L^∞ norm
 on evaluated in the midpoints

in [8]. The position of the interface is given in parametric

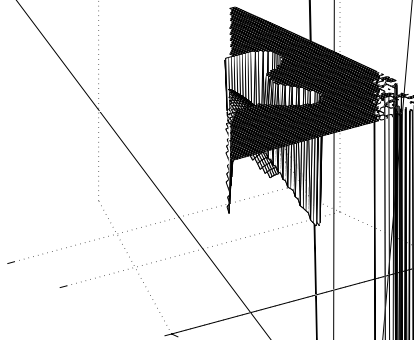
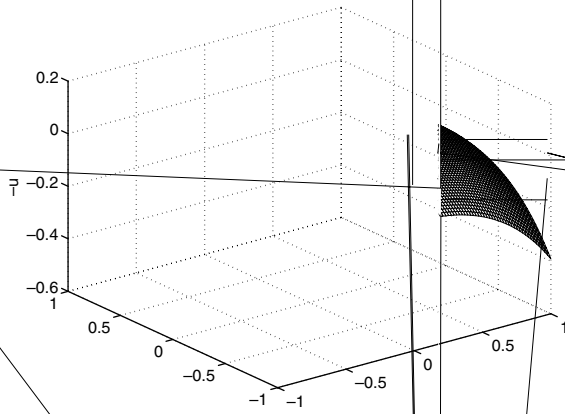
$$r_1 \cos(\omega\theta), \quad 0 \leq \theta \leq 2\pi. \tag{31}$$

parameters are set to $r_0 = 0.5$, $r_1 = 2$, $\omega = 5$, and $x_0 = y_0 = 0.2/\sqrt{20}$.

The analytic solution on the computational domain $-1 \leq x, y \leq 1$ is given as

$$u^+ = \frac{r^4 + C_0 \log(2r)}{\beta^+}, \quad u^- = \frac{r^2}{\beta^-},$$

$$\beta^+ = \text{const.}, \quad \beta^- = \text{const.},$$



where $r = \sqrt{(x - x_0)^2 + (y - y_0)^2}$ and $C_0 = -0.1$. Fig. 12 shows solutions on grids with 100×100 points and convergence results for three different sets of coefficients β^+ , β^- . A characteristic feature of this example is that the solution becomes constants in regions with large β values, which is clearly seen for the second and third case in Fig. 12 with $\beta^+ = 1000$, $\beta^- = 1$ and $\beta^+ = 1$, $\beta^- = 1000$, respectively.

The convergence results in Fig. 12 have been obtained on 30 different meshes having 80×80 up to 1040×1040 grid points. In all three cases we see a sharp drop of the error on the coarsest grids indicating a poorly resolved interface. We left those results out in the evaluation of the convergence rates. The observed convergence rates – or rather the slopes s of the linear least square fit – vary between 2.0–2.2 in the L^2 norm and 1.8–1.9 in the L^∞ norm for the solution values u indicating locally second order of accuracy even for large ratios of the coefficients β^+ and β^- . Furthermore, we observe a strongly non-monotonic behavior of the maximum error I^∞ under grid refinement. This can be explained by the fact that the control points of the interface on a Cartesian grid using a level set approach – namely the points where the interface cuts grid lines – are non-uniformly spaced and that the distribution of those control points might get locally more unequal under grid refinement. Similar behavior has been observed in [8]. As in example 1 we have for the gradient of u an order of accuracy of 1 in the L^∞ norm. In this example we see with values between 1.6 and 1.8 almost second order convergence of the gradient in the L^2 norm. The qualitative similarity between the curves for u and $|\nabla u|$ is apparent.

We repeated the calculations with values of $\beta^+ = 1$, $\beta^- = 10^{-3}$ and $\beta^+ = 10^{-3}$, $\beta^- = 1$. Up to an exact scaling factor of 1000 the results are identical to the investigated set of coefficients $\beta^+ = 1000$, $\beta^- = 1$ and $\beta^+ = 1$, $\beta^- = 1000$, respectively.

4.3. Example 3

In the third example, the interface is again given by Eq. (31) with the following set of parameters: $x_0 = 0.1$, $y_0 = 1.2$, $r_0 = 0.5$, $r_1 = 0.15$, and $\omega = 4$. The solution domain is a square defined by $-1 \leq x \leq 1$ and $0 \leq y \leq 2$. The exact solution is adapted from [8]:

$$\begin{aligned} u^+ &= e^x(x^2 \sin(y) + y^2), \\ u^- &= -(x^2 + y^2). \end{aligned}$$

In contrast to [8] we have varying coefficients

$$\begin{aligned} \beta^+ &= 1000(xy + 5), \\ \beta^- &= 1 + x^2 + y^2. \end{aligned}$$

The maximum ratio β^+/β^- at the interface is about 3600 and the smallest about 1100. Compared to example 2 the solution is independent of the coefficient β . However, the magnitude of the jump $[\beta u_n]$ increases with the jump $[\beta]$.

Fig. 13 shows the numerical solution on a 100×100 grid and convergence results in the L^∞ and L^2 norm. The asymptotic convergence rates for the solution values are 2.1 in the L^2 norm and 1.8 in the L^∞ norm showing again locally second order of accuracy of the method. As in the examples before, we see again an order of accuracy of 1 for the gradient in the L^∞ norm and a slightly better value of 1.5 in the L^2 norm.

4.4. Example 4

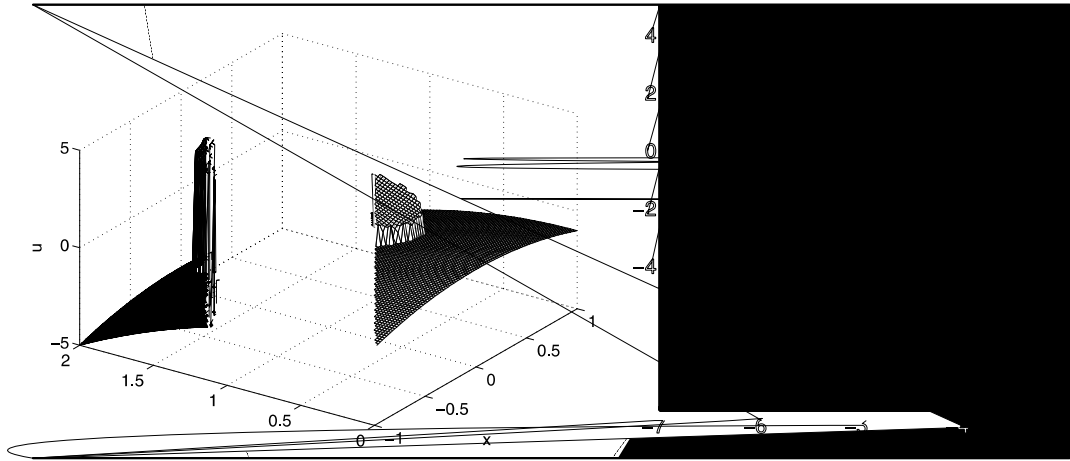
This example is taken from Hou and Liu [4]. The interface is a cardioid with a level set function given by

$$\phi(x, y) = (3(x^2 + y^2) - x)^2 - x^2 - y^2.$$

The specific feature of this example is the singular point of the interface with a cusp point at $x = y = 0$, Fig. 14. The analytic solutions u^\pm , the coefficients β^\pm , and the level set function are given as follows:

$$\begin{aligned} u^+ &= 1 - x^2 - y^2, & u^- &= x^2 + y^2 + 2, \\ \beta^+ &= x^2 - y^2 + 3, & \beta^- &= xy + 3. \end{aligned}$$

Fig. 14 shows the numerical solution on a grid with 100×100 grid points and results of a convergence study on 35 grids ranging from 80×80 to 1040×1040 grid points. Since this is a non-smooth interface at the cusp



point, we cannot expect second order convergence in the L^∞ norm for the solution values of u . The convergence results in Fig. 14 demonstrate second order convergence in the L^∞ norm on the coarser grids comparable to those used by Hou and Liu [4], and first order on finer grids which resolve the cusp. We find second order convergence on all grids in the L^∞ norm if we exclude the area around the cusp point. Corresponding to the abrupt change in the convergence order for the solution u we see an interim increase of the error in the gradient. The overall order of convergence for the gradient in the L^∞ has been evaluated to a value of 0.8 for this problem. The L^2 norm indicates second order convergence on all grids for the solution u and a convergence order of 1.6 for the gradient $|\nabla u|$.

5. Conclusion

We have developed a second-order accurate method for the solution of elliptic equations with variable coefficients and discontinuities across an embedded interface. The interface is represented by a level set approach. In contrast to existing methods in the literature we use a finite volume approach on Cartesian grids using ideas from finite element methods in reconstructing the solution within grid cells. We have presented a piecewise bilinear finite element for irregular cut cells taking into account known jump conditions of the solution and the normal gradient across the interface. We resolve singularities arising from the bilinear ansatz itself and the position of the interface relative to the grid by a two-step asymptotic approach. Although the subject

of this work is the numerical solution of elliptic equations we note that our bilinear finite element might be equally useful for the reconstruction of any other discontinuous function on Cartesian grids (e.g.: the velocity field in premixed combustion). Our discretisation leads to a compact nine-point stencil for the discrete Laplacian, with appropriately adjusted weights near the interface. The resulting set of linear equations is symmetric and positive definite in case of constant and equal coefficients. To be slightly non-symmetric. We have used the black box algebraic multigrid solver of the hypre package [3] as a direct solver or as a preconditioner for the BICGSTAB method to solve the systems of linear equations. Problems of the type considered here become notoriously difficult to solve numerically for limitingly large ratios of the coefficients, say $\beta^+/\beta^- \rightarrow \infty$. We will address this issue systematically, again using asymptotic methods, in a forthcoming publication. The method in principle can be extended to three spatial dimensions where we have four different types of irregular cells and work with piecewise trilinear ansatz functions.

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Appendix A

In Section 3.4.1, Eq. (22), we introduced the matrices \underline{B}_1 and \underline{B}_2 to write $\underline{b}^{(1)}$ in terms of $\underline{x}^{(0)}$ and \underline{b} . The are given in detail here:

$$\underline{B}_1 = (-1) \begin{bmatrix} 0 & \dots & \dots & \dots & \dots & 0 \\ \vdots & & & \ddots & & \vdots \\ 0 & \dots & \dots & \dots & \dots & 0 \\ \frac{1}{\varepsilon} & \frac{1}{\varepsilon} & \frac{a}{\varepsilon} & \frac{a}{\varepsilon} & -\frac{1}{\varepsilon} & 0 & 0 & 0 \\ \frac{1}{\varepsilon} & \frac{b}{\varepsilon} & \frac{-1}{\varepsilon} & \frac{b}{\varepsilon} & -\frac{1}{\varepsilon} & 0 & 0 & 0 \\ \frac{1}{\varepsilon} & \frac{1+b}{\varepsilon} & \frac{1+a}{\varepsilon} & \frac{(1+a)(1+b)}{4\varepsilon} & -\frac{1}{\varepsilon} & 0 & 0 & 0 \\ 0 & \frac{\beta^{\alpha} n_{\xi}}{\Delta x} & \frac{\beta^{\alpha} n_{\eta}}{\Delta y} & \frac{\beta^{\alpha} n_{\xi}(1+a)}{2\Delta x} + \frac{\beta^{\alpha} n_{\eta}(1+b)}{2\Delta y} & 0 & 0 & 0 & 0 \end{bmatrix}$$

and

$$\underline{B}_2 = \begin{bmatrix} 0 & \dots & \dots & \dots & \dots & 0 \\ \vdots & & & \ddots & & \vdots \\ 0 & \dots & \dots & \dots & \dots & 0 \\ 0 & \dots & 0 & \frac{1}{\varepsilon} & 0 & 0 & 0 & 0 \\ \vdots & \ddots & \vdots & 0 & \frac{1}{\varepsilon} & \vdots & \vdots & \vdots \\ & & & \frac{1}{2\varepsilon} & \frac{1}{2\varepsilon} & & & \\ 0 & 0 & 0 & \dots & 0 & \frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

Appendix B

In Section 3.4.2, Eq. (30), we introduced the matrices \underline{B}_1 and \underline{B}_2 to write $\underline{b}^{(1)}$ in terms of $\underline{x}^{(0)}$ and \underline{b} . The are given in detail here:

$$\underline{B}_1 = \left[\begin{array}{cccc|ccc} 0 & \dots & \dots & \dots & & & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & \dots & \dots & \dots & & & 0 \\ -1 & -a & 0 & 0 & 1 & \tilde{a} & 1 & \tilde{a} \\ -1 & -b & -1 & -b & 1 & \tilde{b} & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{4} & 0 & 0 & 0 & \frac{1}{4} \\ 0 & \frac{-\beta^{\alpha} n_{\xi}}{\Delta x} & \frac{-\beta^{\alpha} n_{\eta}}{\Delta y} & \frac{-\beta^{\alpha} n_{\xi}}{2\Delta x} - \frac{\beta^{\alpha} n_{\eta}(a+b)}{2\Delta y} & 0 & \frac{-\beta^{\alpha} n_{\xi}}{\Delta x} & \frac{-\beta^{\alpha} n_{\eta}}{\Delta y} & \frac{-\beta^{\alpha} n_{\xi}}{2\Delta x} - \frac{\beta^{\alpha} n_{\eta}(\tilde{a}+\tilde{b})}{2\Delta y} \end{array} \right]$$

and

$$\underline{\underline{B}}_2 = \begin{bmatrix} 0 & \dots & \dots & \dots & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & \dots & \dots & \dots & 0 \\ 0 & \dots & 0 & 1 & 0 & 0 & 0 \\ \vdots & \ddots & \vdots & 0 & 1 & \vdots & \vdots \\ & & & 0 & 0 & 0 & 0 \\ 0 & \dots & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{bmatrix}.$$

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